

Chemistry 129.01 - General Chemistry Workshop - Spring 2017

Week #5

Monday, February 20. Molecular Polarity, Valence Bond Theory and Hybridization.

Assigned reading: Sections 8.1 – 8.3

Continuing our molecular shape conversation, we'll discuss how to determine if a molecule is polar or nonpolar based on its shape.

Today we are learning about Valence Bond Theory. This is bringing together the ideas behind Lewis Structures and our knowledge of what atomic orbitals look like. By determining the geometry of the molecule, we can then get a better picture of what molecules look like. In other words, our depictions of molecules have so far centered upon sticks (representing bonds) and where the nuclei are in the molecule. Since the nuclei actually occupy very little of the space of the molecule, this depiction is largely erroneous. Valence Bond theory gives a better depiction of where the electrons are in the molecule and how a bond forms.

We start out this discussion by combining atomic orbitals into new orbitals called "Hybrid Orbitals". These orbitals are hybrids between the now familiar s-, p-orbitals and d-orbitals. Read over section 8.2 very carefully. I want you to pay particular attention to Figures 8.9, 8.13, 8.16 and Table 8.21. As you look at Table 8.21, associate the hybridization with a geometry. In addition to molecular shape, we'll also use hybrid orbitals to describe the formation of multiple bonds.

Before Monday's class,

1. Define the following terms:

Hybrid orbital

Sigma bond

2. Take a look at the Lewis structure of acetic acid on page 367 (check your learning), what is the molecular geometry of the two C atoms and the two O atoms?

3. Draw the Lewis structure of a molecule with Trigonal Planar electron-group geometry

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Friday, February 24. Finish Session 8 of GHG Module

Assigned reading: Section 8.4

Quiz today: Orbitals, quantum numbers, electron configurations, periodic properties.

Today and Monday we are talking about Molecular Orbital (MO) theory. This is the highest level of bonding theory that we will learn and it does the best job at explaining experimental data. Unfortunately, the theory is really only manageable (without a computer) for very small molecules. We are going to concentrate solely upon these very simple molecules.

Look carefully at Table 8.2. Valence Bond theory uses hybrid orbitals that belong to one atom to describe bonding in molecules. As shown in figure 8.29, in MO theory, atomic orbitals are combined to form molecular orbitals that are spread over the whole molecule. These molecular orbitals are a probability density map showing the most likely location of the electrons in a molecule (like atomic orbitals in atoms). One of the molecular orbitals is lower in energy (relative to the atomic orbitals) and the other higher in energy.

Read the section (through page 380) carefully, but in particular pay attention to the Figures 8.35 and 8.36. Notice in each MO diagram, that the scheme is about the same, two orbitals come together and form two orbitals. One of the new orbitals goes down in energy (the bonding orbital), and one of the orbitals goes up in energy (the anti-bonding orbital). The names σ and π are merely descriptions of the symmetry of the MO.

Next week will discuss the second period diatomic molecules.

Before Friday's class,

1. Define the following terms:

paramagnetic

molecular orbital

bond order

2. Draw Lewis structure of O_2 . Based on the Lewis structure only, how many unpaired electrons does O_2 have?

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Problem Set #1

Due Monday, February 27 (at the beginning of class). Late homework will not be accepted.

1. Draw their Lewis structure and predict whether the following molecules are polar or nonpolar:
 - a. CS_2
 - b. BrF_5
 - c. BH_3
 - d. CH_4
 - e. XeF_2
 - f. SF_4
2. Even though all three atoms in ozone, O_3 , are the same, it has a small dipole moment. Explain.
3. (a) Draw sketches showing how the following pairs of orbitals (on two different atoms) overlap to form a sigma (σ) bond: two s orbitals, two p orbitals, and one s and one p orbitals.

(b) Draw a sketch showing how the two p orbitals (on two different atoms) overlap to form a pi (π) bond.

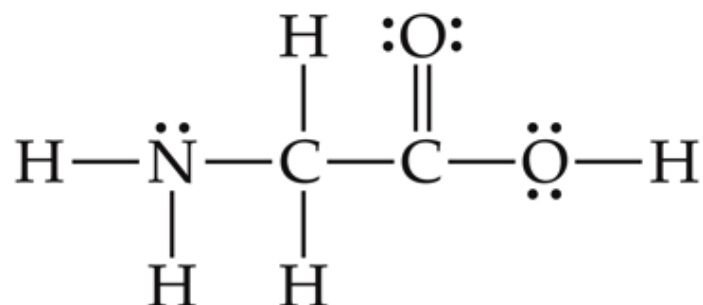
(c) Which is generally stronger a σ bond or a π bond? Explain.

(d) Can two s orbitals make a π bond? Explain.
4. Fill in the following chart. If the molecule column is blank, find an example that fulfills the conditions of the rest of the row.

Molecule	Electron-Group Geometry	Hybridization of Central Atom	Polar? Yes or No.
CO_2			
		sp^3	yes
		sp^3	no
	trigonal planar		no
SF_4			
	octahedral		no
		sp^2	yes
	trigonal bipyramidal		no
XeF_2			

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5. Why are there no sp^4 or sp^5 hybrid orbitals?
6. Draw the Lewis structure of the following molecules and determine the hybridization of the central atom:
- | | |
|--------------|---------------|
| (a) $SiCl_4$ | (d) ICl_2^- |
| (b) HCN | (e) BrF_4^- |
| (c) SO_3 | |
7. The nitrogen atoms in N_2 participate in triple bonding, whereas those in hydrazine, N_2H_4 , do not.
- Draw Lewis structures for both molecules.
 - What is the hybridization of the N atoms in each molecule?
 - Which molecule has a stronger N—N bond?
8. Consider the Lewis structure of glycine, the simplest amino acid:
- What are the hybridizations of the **two carbon** atoms, the **two oxygen** atoms, and the **nitrogen** atom?



- How many sigma bonds and pi bonds does the glycine have?
9. (a) Sketch the molecular orbitals of the H_2^- ion, and draw its energy-level diagram. (b) Write the electron configuration of the ion in terms of its MOs. (c) Calculate the bond order in H_2^- .